Washington University in St. Louis

Washington University Open Scholarship

Volume 12

Washington University Undergraduate Research Digest

Spring 2017

Doping BiI3: A Computational Study of Electronic Properties

Yvette Anguiano
Washington University in St. Louis

Doping BiI_3: A Computational Study of Electronic Properties

Yvette Anguiano

Mentor: Rohan Mishra

Bismuth tri-iodide (BiI_3) has recently been proposed as a photovoltaic material. However, in order to improve the efficiency of BiI_3 based photovoltaics, suitable dopants need to be identified. We have used density functional theory calculations to study the electronic properties of BiI_3 with substituent dopants at either the bismuth or the iodine site. Based on the density of states calculations, we predict, Ti and Zr are potential *n*-type dopants substituting Bi with contributions to the conduction band minimum and Ni is a potential *p*-type candidate with contributions to the valence band maximum. For substitution at the iodine site, we examined Sb and Te, and they were found to be suitable *p*-type dopants.